

Comparison of the Effective Interaction to Various Orders in Different Mass Regions

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Abstract

The convergence of the perturbation expansion for the effective interaction to be used in shell-model calculations is investigated as function of the mass number A , from $A = 4$ to $A = 208$. As the mass number increases, there are more intermediate states to sum over in each higher-order diagram which contributes to the effective interaction. Together with the fact that the energy denominators in each diagram are smaller for larger mass numbers, these two effects could largely enhance higher-order contributions to the effective interaction, thereby deteriorating the order-by-order convergence of the effective interaction. This effect is counterbalanced by the short range of the nucleon-nucleon interaction, which implies that its matrix elements are weaker for valence single-particle states in “large” nuclei with large mass number as compared to those in light nuclei. These effects are examined by comparing various mean values of the matrix elements. It turns out that the contributions from higher-order terms remain fairly stable as the mass number increases from $A = 4$ to $A = 208$. The implications for nuclear structure calculations are discussed.

PACS number(s): 21.60.-n, 24.10.Cn

I. INTRODUCTION

One of the long-standing problems in nuclear many-body theory has been the convergence of the perturbative expansion for the effective interaction H_{eff} (or equally well that of effective operators) derived from realistic nuclear forces to be used in nuclear structure calculations. Conventionally, the various terms which appear in a perturbative expansion for H_{eff} are displayed by way of Feynman-Goldstone diagrams, examples of such diagrams are shown in Fig. 1. It is well known that a realistic nucleon-nucleon interaction V_{NN} contains strong components of short range, which renders a perturbative expansion in terms of V_{NN} meaningless. To overcome this problem, one takes into account the short-range correlations through the solution of the Bethe-Brueckner-Goldstone equation and considers a perturbation in terms of the nuclear reaction matrix G . The wavy lines in Fig. 1 represent such G interactions. However, higher-order perturbative contributions in terms of the G -matrix, may be large, and the convergence of the perturbative expansion slow or not convergent at all. Actually, Barrett and Kirson [1] showed that third-order contributions to the effective interaction were substantial, and raised the question whether the perturbative Rayleigh-Schrödinger (RS) expansion in terms of the nuclear G -matrix did converge at all. Schucan and Weidenmüller [2] even pointed out that the order-by-order expansion of the effective interaction will ultimately diverge when so-called intruder states are present. Typical intruder states for nuclei like ^{18}O and ^{42}Ca are four-particle-two-hole core-deformed states. It ought however to be mentioned that for nuclei with more valence nucleons in e.g. the oxygen mass area, such intruder state configurations may not be important, and a two-body (or many-body) effective interaction defined within the $1s0d$ -shell only, may represent the relevant degrees of freedom.

Most microscopic investigations of H_{eff} have been performed for nuclei in the $1s0d$ -shell, with few valence nucleons outside a ^{16}O core. However, when one extends the area of investigation to nuclei in the mass regions of calcium, tin or lead, one has to face the problem that for diagrams like those displayed in Fig. 1, there are more intermediate states which

contribute to each diagram of the effective interaction in e.g. the $1p0f$ -shell than in the $1s0d$ -shell. Moreover, the energy spacing between the various major shells is also smaller for nuclei in the $1p0f$ -shell than for those around ^{16}O . This leads to smaller energy denominators which should enhance third-order or higher-order contributions. Thus, the combined action of the above effects could seriously deteriorate the order-by-order convergence (if it does converge) of the effective interaction. The only mechanism which could quench these effects, is the fact that the matrix elements of G calculated in the $1p0f$ -shell should in general be weaker than those in the $1s0d$ -shell. The single-particle wave functions for the states around the Fermi energy exhibit larger radii and, as the nucleon-nucleon interaction is of short range, the matrix elements of G should be weaker for the heavier nuclei. The same arguments apply of course as well for the tin and lead regions.

It is then the scope of this work to study the convergence of the effective interaction in terms of the mass number A , in order to assess whether higher-order contributions to the two-body effective interaction decrease or increase as A increases. To achieve this, we calculate all non-folded valence linked diagrams through third-order in the interaction G , and sum higher-order folded diagrams to infinite order for the mass regions beyond closed-shell cores with $A = 4$, $A = 16$, $A = 40$, $A = 100$ and $A = 208$. The details on how to obtain these effective interactions are briefly sketched in the next section, together with our results and discussions. Some concluding remarks are given in section three.

II. COMPUTATIONAL DETAILS AND RESULTS

There are basically two main approaches in perturbation theory used to define an effective operator and effective interaction, each with its hierarchy of sub-approaches. One of these main approaches is an energy-dependent approach, known as Brillouin-Wigner perturbation theory, while the Rayleigh-Schrödinger (RS) perturbation expansion stands for the energy independent approach. The latter is the most commonly used approach in the literature [3,4], an approach which we will also employ here. It is then common practice in

perturbation theory to reduce the infinitely many degrees of freedom of the Hilbert space to those represented by a physically motivated subspace, the shell-model valence space. In such truncations of the Hilbert space, the notions of a projection operator P on the model space and its complement Q are introduced. The projection operators defining the model and excluded spaces are defined by

$$P = \sum_{i=1}^D |\psi_i\rangle \langle\psi_i|, \quad (1)$$

and

$$Q = \sum_{i=D+1}^{\infty} |\psi_i\rangle \langle\psi_i|, \quad (2)$$

with D being the dimension of the model space, and $PQ = 0$, $P^2 = P$, $Q^2 = Q$ and $P + Q = I$. The wave functions $|\psi_i\rangle$ are eigenfunctions of the unperturbed hamiltonian $H_0 = T + U$ (with eigenvalues ε_i), where T is the kinetic energy and U an appropriately chosen one-body potential, in this work that of the harmonic oscillator (h.o.). The oscillator energies $\hbar\Omega$ will be derived from $\hbar\Omega = 45A^{-1/3} - 25A^{-2/3}$, A being the mass number. This yields $\hbar\Omega = 18.4$, $\hbar\Omega = 13.9$, $\hbar\Omega = 11.0$, $\hbar\Omega = 8.5$ and $\hbar\Omega = 6.9$ MeV for $A = 4$, $A = 16$, $A = 40$, $A = 100$ and $A = 208$, respectively. The full hamiltonian is then rewritten as $H = H_0 + H_1$ with $H_1 = V_{\text{NN}} - U$, V_{NN} being the nucleon-nucleon (NN) interaction. Below we will replace V_{NN} by the G -matrix, which will be used as the starting point for our perturbative treatment.

Following the above philosophy, we choose the model spaces which are believed, from both experiment and theoretical calculations, to be relevant for calculations of particle-particle effective interactions in the mass areas from $A = 4$ to $A = 208$. These are the $0p_{3/2}$ and $0p_{1/2}$ orbits for H_{eff} in the mass area of $A = 4$, the $0d_{5/2}$, $0d_{3/2}$ and $1s_{1/2}$ orbits for $A = 16$, the $1p_{3/2}$, $1p_{1/2}$, $0f_{7/2}$ and $0f_{5/2}$ orbits for nuclei in the mass region of $A = 40$ and the $0h_{11/2}$, $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$ and $2s_{1/2}$ orbits for $A = 100$. For these systems, the closed-shell cores (${}^4\text{He}$, ${}^{16}\text{O}$, ${}^{40}\text{Ca}$ and ${}^{100}\text{Sn}$) have equal numbers of protons and neutrons, and the model spaces are the same for both protons and neutrons. For lead however, with

$Z = 82$ and $N = 126$, the proton and neutron model spaces are different, i.e. the orbits $0i_{13/2}$, $0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$ and $2p_{1/2}$ for the proton model space and $0i_{11/2}$, $0j_{15/2}$, $1g_{9/2}$, $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$ and $3s_{1/2}$ for the neutron model space. Since the effective interaction theory we will employ is tailored to degenerate model spaces, we will make no attempt to derive for lead an effective proton-neutron interaction for these two model spaces. Moreover, as discussed in Ref. [5], a multishell effective interaction may show strong non-hermiticities, or even divergencies if a h.o. basis is used. Thus, for $A = 4$ to $A = 100$ we will discuss both isospin $T = 0$ and $T = 1$ effective interactions, whereas for lead we restrict the attention to $T_z = -1$ and $T_z = 1$, where T_z is the projection of the total isospin.

For the above model spaces, there are in total 15 matrix elements for the effective interaction of $A = 4$, 63 for $A = 16$, 195 for $A = 40$, 353 for $A = 100$, 711 for the neutron model space of $A = 208$ and 353 for the proton model space of $A = 208$. The effective interactions for $A = 16$, $A = 40$ and $A = 100$ are listed in Ref. [5], and have been tested in nuclear structure calculations and a good agreement with the experimental data obtained for several isotopes in these mass areas. The spectra for isotopes in the lead region will be published elsewhere [6].

Having defined the various model spaces, the next step in our calculation is to obtain the nuclear reaction matrix G , given by

$$G = V_{\text{NN}} + V_{\text{NN}} \frac{\tilde{Q}}{\omega - H_0} G, \quad (3)$$

where ω is the unperturbed energy of the interacting nucleons, and H_0 is the unperturbed hamiltonian. For the bare NN interaction we use the One-Boson-Exchange potential Bonn A defined in Table A.1 of Ref. [8]. The operator \tilde{Q} is a projection operator which prevents the interacting nucleons from scattering into states occupied by other nucleons. Note that the exclusion operator used in the calculation of the G -matrix in this work is different from the Q operator used in the evaluation of the effective interaction. The definition of the Pauli operator for the G -matrix can be found in Refs. [5,7], where the so-called double-partitioned scheme has been used. This means that low-lying two-particle states are excluded by \tilde{Q} from

the intermediate states in the Bethe-Goldstone Eq. (3). For the example of the $1s0d$ -shell this exclusion refers to states with two nucleons in the $1p0f$ -shell. As a consequence, we have to include in our perturbation expansion ladder type diagrams, such as (2-3) in Fig. 1, where the allowed intermediate states are those of the $1p0f$ -shell or corresponding ones for the other model-spaces.

The next step is to define the so-called \hat{Q} -box¹ given by

$$P\hat{Q}P = PH_1P + P \left(H_1 \frac{Q}{\omega - H_0} H_1 + H_1 \frac{Q}{\omega - H_0} H_1 \frac{Q}{\omega - H_0} H_1 + \dots \right) P, \quad (4)$$

where we will replace H_1 with G (G replaces the free NN interaction V_{NN}). The \hat{Q} -box is made up of non-folded diagrams which are irreducible and valence linked. A diagram is said to be irreducible if between each pair of vertices there is at least one hole state or a particle state outside the model space. In a valence-linked diagram the interactions are linked (via fermion lines) to at least one valence line. Note that a valence-linked diagram can be either connected (consisting of a single piece) or disconnected. In the final expansion including folded diagrams as well, the disconnected diagrams are found to cancel out [3]. This corresponds to the cancellation of unlinked diagrams in the Goldstone expansion [3].

We can then obtain an effective interaction $H_{\text{eff}} = H_0 + V_{\text{eff}}$ in terms of the \hat{Q} -box, with [3,5]

$$V_{\text{eff}}^{(n)} = \hat{Q} + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} \left\{ V_{\text{eff}}^{(n-1)} \right\}^m. \quad (5)$$

Observe also that the effective interaction $V_{\text{eff}}^{(n)}$ is evaluated at a given model space energy ω , as is the case for the G -matrix as well. For all mass areas, we fix $\omega = -20$ MeV. The first iteration is then given by

$$V_{\text{eff}}^{(0)} = \hat{Q}. \quad (6)$$

In this work we define the \hat{Q} -box to consist of all diagrams through third order in the G -matrix, as discussed in Ref. [5]. Less than ten iterations were needed in order to obtain a

¹Not to be confused with the Pauli operators Q of the effective interaction and the G -matrix \tilde{Q} .

converged effective interaction for the various values of A . For further details, see Ref. [5]. In the calculation of the various diagrams, we limit the intermediate state excitations to $2\hbar\omega$ in oscillator energy, an approximation which is viable if one employs an NN potential with a weak tensor force (such as the Bonn potential used here), as discussed by Sommermann *et al.* [9]. It is the aim of this study to explore the effects of the various contributions to V_{eff} . As it will be rather confusing to discuss the effects for individual matrix elements (recall that depending on the model-space there are up to few hundred matrix elements), we define averages of matrix elements by

$$\langle O \rangle_{\text{diag}} = \frac{\sum_j \sum_{JT} (2J+1)(2T+1) \langle j | O | j \rangle_{JT}}{\sum_j \sum_{JT} (2J+1)(2T+1)}, \quad (7)$$

where the summation index j refers to all two-particle states of the model-space under consideration, coupled to angular momentum J and isospin T ². In the averaging procedure defined in this equation we have weighted the matrix elements by the factor $(2J+1)(2T+1)$ since this factor accounts for the degeneracy of two-particle states with respect to the projection quantum numbers and occurs e.g. in the calculation of the energy if all valence states are occupied. It turned out, however, that the main features of the results discussed below are obtained as well, if this weighting factor is dropped. For the operator O we will consider $V^{(1)}$, which corresponds to the bare G matrix, Q^2 , the \hat{Q} -box including terms up to second order in G without folded diagrams, and $V^{(2)}$ ($V^{(3)}$) the effective interaction including all \hat{Q} -box diagrams up to second (third) order plus all folded diagrams derived from these \hat{Q} -boxes. Note, that the average defined in Eq. (7) includes only diagonal matrix elements. In order to study if the conclusions remain valid for all matrix elements we also define a mean value including all matrix elements by

²In tables I and II we omit to divide with the number of configurations, as this gives rather small numbers for the heavier nuclei.

$$\langle O \rangle = \frac{\sum_{kl} \sum_{JT} (2J+1)(2T+1) \langle k | O | l \rangle_{JT}}{\sum_{kl} \sum_{JT} (2J+1)(2T+1)}, \quad (8)$$

where the summation indices k and l include again all two-particle states of the model-space considered. Beside these averages, which include matrix elements of isospin $T = 0$ and $T = 1$, we will also report on results where the averaging is restricted to one of these isospins only.

Results for the mean values of diagonal matrix elements (see Eq. (7)) are listed in table I, while averages including the non-diagonal matrix elements as well (see Eq. (8)) are presented in table II for the various model-spaces considered.

Inspecting these tables one observes very clearly that the mean values for the matrix elements are getting less attractive for the model spaces referring to heavy nuclei. This trend can be observed independent on the approximation used to calculate V_{eff} . This behavior reflects the fact that also the effective interaction, calculated with inclusion of higher order terms, is of short range and therefore, as we discussed already above, yield weaker matrix elements for the valence nucleons in heavy nuclei as compared to the light systems.

Furthermore, we observe some features which are valid independent on the mass number and model space considered:

- The inclusion of second-order \hat{Q} -box diagrams in $Q^{(2)}$ yields a substantial attraction for the $T = 0$ matrix elements and a repulsion for $T = 1$. This difference may be understood by the following argument: For the $T = 1$ channel, the major mechanism which accounts for the difference between first and second order, is provided by the core-polarization diagram in (2-2) of Fig. 1. Moreover, in the $T = 1$ channel, the tensor force component of the nucleon-nucleon interaction is not so important, whereas in the $T = 0$ channel the contribution from the 3S_1 - 3D_1 partial wave plays an important role in ladder-type diagrams, such as several of the folded diagrams, or the particle-particle ladder diagram in (2-3) of Fig. 1. Typically, for many $J = 1$ and $T = 0$ particle-particle effective interactions, the particle-particle ladder is of the size of or larger than the

core-polarization diagram, while for $J = 0$ and $T = 1$, the core-polarization diagram and the G -matrix yield the largest contribution to the effective interaction.

- The inclusion of folded diagrams yields a repulsive trend going from $Q^{(2)}$ to $V^{(2)}$. The effect is again much larger in the $T = 0$ than in the $T = 1$ matrix elements, which can as well be understood from the importance of the particle-particle ladder diagrams in the $T = 0$ states. Comparing the results of $V^{(1)}$ and $V^{(2)}$ one observes a repulsion for both isospins.
- Contrary to this repulsion due to the second-order terms in the folded-diagram expansion, the additional inclusion of terms of third order in G yields some attraction in $V^{(3)}$ as compared to $V^{(2)}$. Except for the case of ${}^4\text{He}$, the effect of third-order terms is very weak for the $T = 1$ states. This was also observed in Ref. [5] in the study of the spectra of nuclei with valence particles being only neutrons or protons. There the authors noted that the spectra of e.g. ${}^{18}\text{O}$ or ${}^{42}\text{Ca}$ obtained with either a second-order or third-order effective interaction were quite similar. For calculations of the effective interaction for lead or tin, this is a gratifying property since it means that one needs only to evaluate the \hat{Q} -box to second order and sum all folded diagrams.

Finally, in order to discuss the convergence of the perturbation expansion, we compare in table III the ratios evaluated from the mean values defined in Eq. (7). These ratios reflect of course the same features which we already discussed above. They emphasize, however, in a much better way that the different ratios are rather insensitive on the mass number which is considered. This means that one can expect the convergence of the perturbation expansion for the residual interaction to be as good (or bad) for heavy nuclei as for the light nuclei around ${}^{16}\text{O}$, which are usually studied.

For nuclear structure studies of heavy nuclei with neutron numbers quite different from the proton number one typically considers model-spaces, which are separate for protons and neutrons, ignoring the residual interaction beyond the mean-field approximation. For these cases (isospin $T = 1$), the effects of terms of second order in G seem to be rather important

with $V^{(2)}$ containing a correction of around 50 percent of the average of $V^{(1)}$. However, it is encouraging to note that the inclusion of third order terms yields a correction of only 5 percent or even below.

III. CONCLUSIONS

We have studied the behavior of the perturbation expansion for the effective interaction to be used in shell-model studies of nuclei with various mass numbers. Inspecting appropriate mean values of matrix elements, we have found that the fact that the G -matrix becomes smaller in absolute value with increasing mass numbers, counterbalances the effects that there are more intermediate states to sum over and that the energy denominators become smaller in each individual diagram of the effective interaction. Therefore, the convergence of the perturbation expansion seems to be rather insensitive to the nuclear mass number. We observe that various features of the folded-diagram expansion, which had been discussed for the mass region $A \approx 16$, can also be found in heavy nuclei. The nuclear structure calculations for heavy nuclei are mainly sensitive to the proton-proton and neutron-neutron residual interactions. For these $T = 1$ matrix elements the third-order and second-order averages are very close, indicating that for this isospin channel one can approximate the effective interaction by including all diagrams to second order plus folded diagrams to all orders. For $T = 0$, one still needs to account for third-order contributions.

The fact that third-order contributions seem to stabilize for heavier nuclei, has also important consequences for nuclear structure calculations in nuclei in the mass regions of e.g. ^{132}Sn and ^{208}Pb . This means that the methods used to calculate the effective interaction for valence nucleons, applied mainly in the mass regions of ^{16}O and ^{40}Ca , can be applied to the mass regions of ^{132}Sn and ^{208}Pb , as done recently in Refs. [6,10].

We gratefully acknowledge the financial support of the NorFA (Nordic Academy for Advanced Study), grant 93.40.018/00. One of us, MHJ, thanks the Istituto Trentino di Cultura, Italy and the Research Council of Norway for their support.

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TABLES

TABLE I. The mean values for diagonal matrix elements calculated according to Eq. (7) in model-spaces with cores as indicated in the first row assuming various approximations for the effective interaction. Averages are listed for all isospins (\sum_T) as well as for $T = 0$ ($\sum_{T=0}$) and $T = 1$ ($\sum_{T=1}$). For lead, results for averages in the proton-proton model-space (\sum_{pp}) and the neutron-neutron model-space (\sum_{nn}) are listed. All entries in MeV.

	\sum_T	$\sum_{T=0}$	$\sum_{T=1}$
${}^4\text{He}$			
$\langle V^{(1)} \rangle$	-3.42	-5.98	-2.23
$\langle Q^{(2)} \rangle$	-3.38	-7.04	-1.68
$\langle V^{(2)} \rangle$	-2.87	-5.85	-1.48
$\langle V^{(3)} \rangle$	-3.42	-7.21	-1.65
${}^{16}\text{O}$			
$\langle V^{(1)} \rangle$	-1.39	-2.67	-0.88
$\langle Q^{(2)} \rangle$	-1.24	-3.10	-0.50
$\langle V^{(2)} \rangle$	-0.99	-2.39	-0.43
$\langle V^{(3)} \rangle$	-1.11	-2.80	-0.44
${}^{40}\text{Ca}$			
$\langle V^{(1)} \rangle$	-0.68	-1.35	-0.43
$\langle Q^{(2)} \rangle$	-0.58	-1.57	-0.21
$\langle V^{(2)} \rangle$	-0.45	-1.20	-0.18
$\langle V^{(3)} \rangle$	-0.53	-1.51	-0.17
${}^{100}\text{Sn}$			

$\langle V^{(1)} \rangle$	-0.28	-0.57	-0.17
$\langle Q^{(2)} \rangle$	-0.23	-0.61	-0.10
$\langle V^{(2)} \rangle$	-0.19	-0.48	-0.08
$\langle V^{(3)} \rangle$	-0.21	-0.57	-0.07
^{208}Pb		\sum_{pp}	\sum_{nn}
$\langle V^{(1)} \rangle$		-0.09	-0.06
$\langle Q^{(2)} \rangle$		-0.04	-0.04
$\langle V^{(2)} \rangle$		-0.04	-0.03
$\langle V^{(3)} \rangle$		-0.04	-0.03

TABLE II. Mean values for diagonal and non-diagonal matrix elements calculated according to Eq. (8). Further details see caption of table I

	\sum_T	$\sum_{T=0}$	$\sum_{T=1}$
^4He			
$\langle V^{(1)} \rangle$	-2.56	-3.06	-2.32
$\langle Q^{(2)} \rangle$	-2.59	-3.56	-2.13
$\langle V^{(2)} \rangle$	-2.21	-2.95	-1.84
$\langle V^{(3)} \rangle$	-2.61	-3.69	-2.09
^{16}O			
$\langle V^{(1)} \rangle$	-0.72	-1.13	-0.56
$\langle Q^{(2)} \rangle$	-0.68	-1.29	-0.44
$\langle V^{(2)} \rangle$	-0.54	-0.99	-0.36
$\langle V^{(3)} \rangle$	-0.59	-1.16	-0.37
^{40}Ca			
$\langle V^{(1)} \rangle$	-0.28	-0.41	-0.22
$\langle Q^{(2)} \rangle$	-0.27	-0.48	-0.19
$\langle V^{(2)} \rangle$	-0.21	-0.36	-0.15
$\langle V^{(3)} \rangle$	-0.23	-0.46	-0.14
^{100}Sn			
$\langle V^{(1)} \rangle$	-0.13	-0.30	-0.07
$\langle Q^{(2)} \rangle$	-0.12	-0.33	-0.04
$\langle V^{(2)} \rangle$	-0.09	-0.26	-0.04
$\langle V^{(3)} \rangle$	-0.11	-0.30	-0.04

^{208}Pb	Σ_{pp}	Σ_{nn}
$\langle V^{(1)} \rangle$	-0.03	-0.02
$\langle Q^{(2)} \rangle$	-0.01	-0.01
$\langle V^{(2)} \rangle$	-0.01	-0.01
$\langle V^{(3)} \rangle$	-0.01	-0.01

TABLE III. Ratios of mean values for diagonal matrix elements calculated according to Eq. (7). These ratios have been evaluated from mean values with better precision than those listed in table I.

	$\langle V^{(2)} \rangle / \langle V^{(1)} \rangle$	$\langle V^{(3)} \rangle / \langle V^{(2)} \rangle$
${}^4\text{He}$		
\sum_T	0.84	1.19
$\sum_{T=0}$	0.98	1.23
$\sum_{T=1}$	0.66	1.11
${}^{16}\text{O}$		
\sum_T	0.71	1.13
$\sum_{T=0}$	0.90	1.17
$\sum_{T=1}$	0.49	1.02
${}^{40}\text{Ca}$		
\sum_T	0.66	1.18
$\sum_{T=0}$	0.89	1.26
$\sum_{T=1}$	0.42	0.94
${}^{100}\text{Sn}$		
\sum_T	0.68	1.11
$\sum_{T=0}$	0.85	1.19
$\sum_{T=1}$	0.49	0.94
${}^{208}\text{Pb}$		
\sum_{pp}	0.44	1.00

Σ_{nn}

0.50

1.00

FIGURES

FIG. 1. Different types of valence-linked diagrams. Diagram (2-1) is the G -matrix, diagrams (2-2)-(2-4) are second-order terms in G , while diagrams (2-5)-(2-8) are examples of third-order diagrams.

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